OF MINNESOTA TWIN CITIES

Efficient Linear Algebra methods for Data Mining

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Team members involved in this work – Support

Past:

• Efi Kokiopoulou [Now at the U. of Lausanne]

Current:

- Jie Chen [grad student]
- Sofia Sakellaridi [grad student]
- Haw-Ren Fang [Post-Doc]

Support:

National Science Foundation

Introduction, background, and motivation

Common goal of data mining methods: to extract meaningful information or patterns from data. Very broad area – includes: data analysis, machine learning, pattern recognition, information retrieval, ...

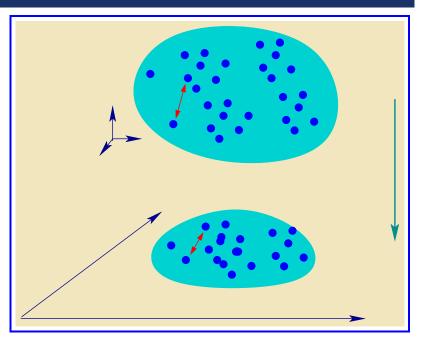
Main tools used: linear algebra; graph theory; approximation theory; optimization; ...

In this talk: emphasis on dimension reduction techniques and the interrelations between techniques

- Focus on two main problems
- Information retrieval
- Face recognition
- and 3 types of dimension reduction methods
- Standard subspace methods [SVD, Lanczos]
- Graph-based methods
- multilevel methods

The problem

- \blacktriangleright Given $d \ll m$ find a mapping
- $\Phi: x \ \in \mathbb{R}^m \longrightarrow y \ \in \mathbb{R}^d$
- Mapping may be explicit (e.g., $y = V^T x$)
- Or implicit (nonlinear)



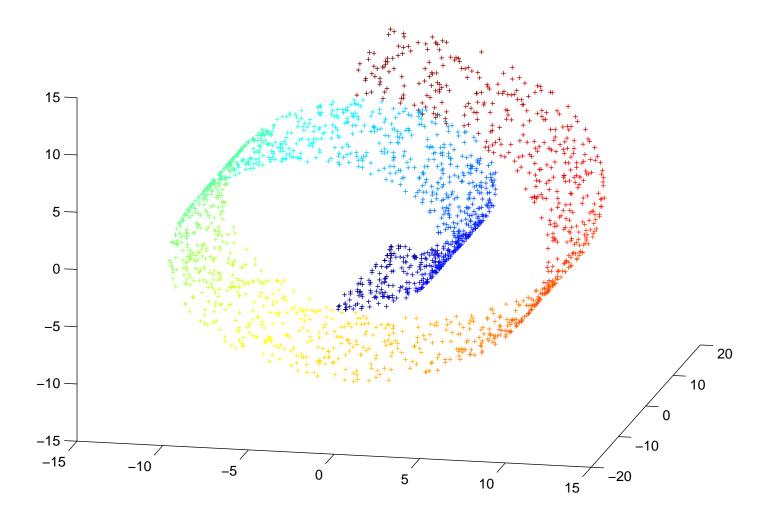


Given $X \in \mathbb{R}^{m \times n}$, we want to find a low-dimensional representation $Y \in \mathbb{R}^{d \times n}$ of X

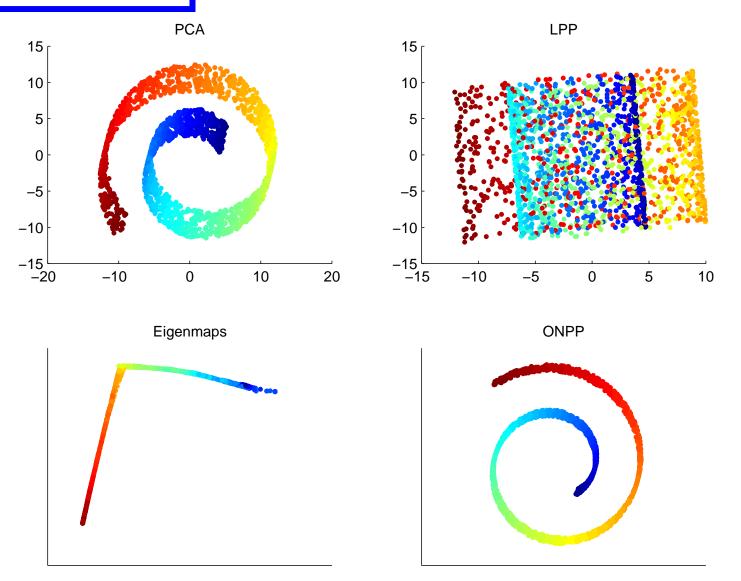
Two classes of methods: (1) projection techniques and (2) nonlinear implicit methods.

Example 1: The 'Swill-Roll' (2000 points in 3-D)

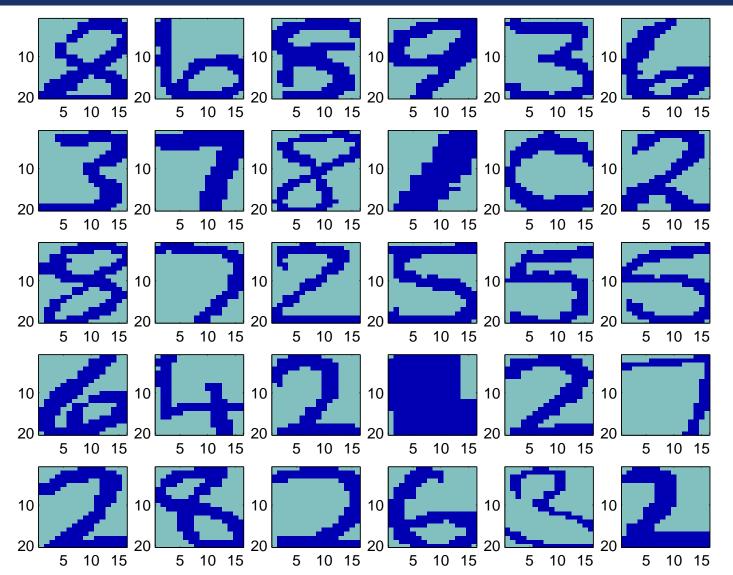
Original Data in 3-D



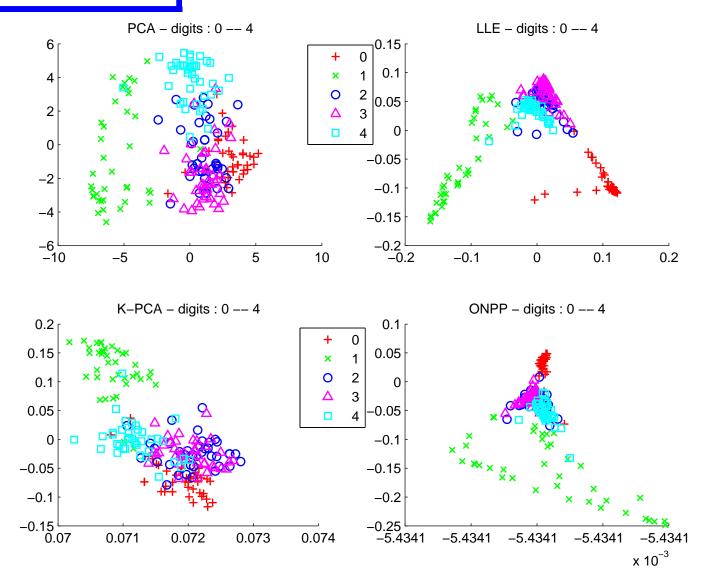
2-D 'reductions':



Example 2: Digit images (a sample of 30)



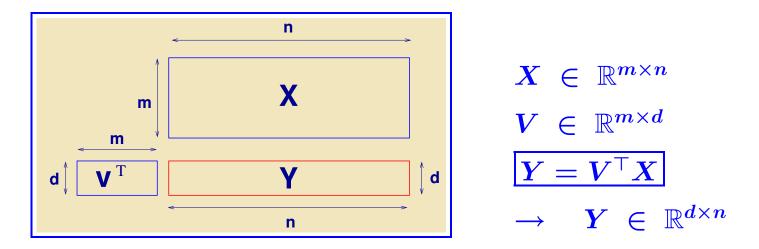
2-D 'reductions':



Projection-based Dimensionality Reduction

Given: a data set $X = [x_1, x_2, ..., x_n]$, and *d* the dimension of the desired reduced space *Y*.

Want: a linear transformation from X to Y



m-dimens. objects (x_i) 'flattened' to *d*-dimens. space (y_i)
 Constraint: The y_i's must satisfy certain properties
 Optimization problem

Linear Dimensionality Reduction: PCA

> In PCA projected data must have maximum variance, i.e., we need to maximize over all orthogonal $m \times d$ matrices V:

$$\sum_i \|y_i - rac{1}{n} \sum_j y_j\|_2^2 = \dots = \mathsf{Tr} \left[V^ op ar{X} ar{X}^ op V
ight]$$

Where: $\bar{X} = X(I - \frac{1}{n}\mathbf{1}\mathbf{1}^T) ==$ origin-recentered version of X

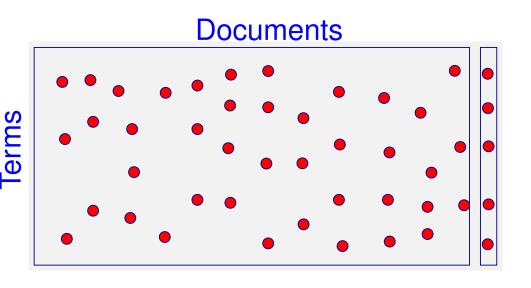
- Solution $V = \{$ dominant eigenvectors $\}$ of the covariance matrix
- == Set of left singular vectors of \bar{X}
- Solution V also minimizes 'reconstruction error' ..

$$\sum_i \|x_i - VV^T x_i\|^2 = \sum_i \|x_i - Vy_i\|^2$$

> .. and it also maximizes [Korel and Carmel 04] $\sum_{i,j} \|y_i - y_j\|^2$

Information Retrieval: Vector Space Model

Given: 1) set of documents (columns of a matrix A); 2) a query vector q. Entry a_{ij} of A = frequency of term i in document j + weighting.



Queries ('pseudo-documents') q represented similarly to columns *Problem:* find columns of A that best match q

Vector Space Model and the Truncated SVD

Similarity metric: angle between column $A_{j,:}$ and query q

Use Cosines:
$$|q^T A_{:,j}|$$

 $||A_{:,j}||_2 ||q||_2$

To rank all documents compute the similarity vector:

$$s = A^T q$$

- Not very effective. Problems : polysemy, synonymy, ...
- LSI: replace matrix A by low rank approximation

$$A = U \Sigma V^T \quad o \quad A_k = U_k \Sigma_k V_k^T \quad o \quad s_k = A_k^T q$$

- \succ U_k : term space, V_k : document space.
- Called TSVD Expensive, hard to update, ..

New similarity vector:

$$s_k = A_k^T q = V_k \Sigma_k U_k^T$$

$\blacktriangleright How to select k?$



- Computational cost (memory + computation)
- Problem with updates

- Alternative: SDD; Less memory but cost still an issue.
- > Alternative: polynomial approximation. $s_k \approx \phi_k(A^T A) A^T q$ where
- $\phi_k = \deg. k \text{ polynom.}$
- Yet another alternative: use Lanczos vectors instead of singular vectors [Ruhe and Blom, 2005]

IR: Use of the Lanczos algorithm

* Joint work with Jie Chen

Lanczos is good at catching large (and small) eigenvalues: can compute singular vectors with Lanczos, & use them in LSI

Can do better: Use the Lanczos vectors directly for the projection..

First advocated by: K. Blom and A. Ruhe [SIMAX, vol. 26, 2005]. Use Lanczos bidiagonalization.

> Use a similar approach – But directly with AA^T or A^TA .

IR: Use of the Lanczos algorithm (1)

► Let $A \in \mathbb{R}^{m \times n}$. Apply the Lanczos procedure to $M = AA^T$. Result:

$$Q_k^T A A^T Q_k = T_k$$

with Q_k orthogonal, T_k tridiagonal.

▶ Define $s_i \equiv$ orth. projection of Ab on subspace span $\{Q_i\}$

 $s_i := Q_i Q_i^T A b.$

> s_i can be easily updated from s_{i-1} :

$$s_i = s_{i-1} + q_i q_i^T A b.$$

IR: Use of the Lanczos algorithm (2)

► If n < m it may be more economial to apply Lanczos to $M = A^T A$ which is $n \times n$. Result:

$$ar{Q}_k^T A^T A ar{Q}_k = ar{T}_k$$

► Define:

$$t_i:=Aar{Q}_iar{Q}_i^Tb,$$

> Project b first before applying A to result.

Why does this work?

First, recall a result on Lanczos algorithm [YS 83]

$$\begin{array}{l} \text{Let } \{\lambda_j, u_j\} = j\text{-th eigen-pair of } M \text{ (label } \downarrow) \\ \\ \frac{\|(I-Q_kQ_k^T)u_j\|}{\|Q_kQ_k^Tu_j\|} \leq \frac{K_j}{T_{k-j}(\gamma_j)} \frac{\|(I-Q_1Q_1^T)u_j\|}{\|Q_1Q_1^Tu_j\|}, \end{array} \end{array}$$

where

$$\gamma_j = 1 + 2rac{\lambda_j - \lambda_{j+1}}{\lambda_{j+1} - \lambda_n}, \qquad K_j = egin{cases} 1 & j = 1 \ \prod_{i=1}^{j-1} rac{\lambda_i - \lambda_n}{\lambda_i - \lambda_j} & j
eq 1 \end{cases},$$

and $T_l(x)$ = Chebyshev polynomial of 1st kind of degree *l*.

This has the form

$$\|(I-Q_kQ_k^T)u_j\|\leq c_j/T_{k-j}(\gamma_j),$$

where c_j = constant independent of k

► Result: Distance between unit eigenvector u_j and Krylov subspace span(Q_k) decays fast (for small j)

Consider component of difference between $Ab - s_k$ along left singular directions of A. If $A = U\Sigma V^T$, then u_j 's (columns of U) are eigenvectors of $M = AA^T$. So:

$$egin{aligned} |\langle Ab-s_k,u_j
angle| &= \left|\langle (I-Q_kQ_k^T)Ab,u_j
angle
ight| \ &= \left|\langle (I-Q_kQ_k^T)u_j,Ab
ight
angle| \ &\leq \|(I-Q_kQ_k^T)u_j\|\|Ab\| \ &\leq c_j\|Ab\|T_{k-j}^{-1}(\gamma_j) \end{aligned}$$

> $\{s_i\}$ converges rapidly to Ab in directions of the major left singular vectors of A.

> Similar result for left projection sequence t_j

► Here is a typical distribution of eigenvalues of M: [Matrix of size 1398×1398]



Convergence toward first few singular vectors very fast –

Advantages of Lanczos over polynomial filters:

- (1) No need for eigenvalue estimates
- (2) Mat-vecs performed only in preprocessing

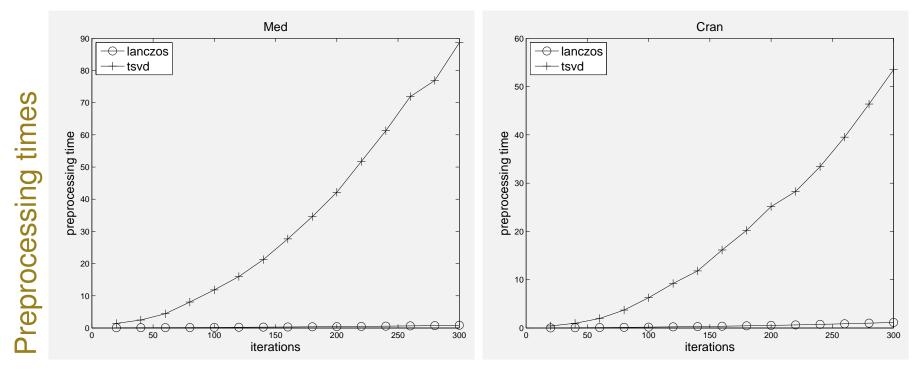
Disadvantages:

- (1) Need to store Lanczos vectors;
- (2) Preprocessing must be redone when A changes.
- (3) Need for reorthogonalization expensive for large k.

Information		# Terms	# Docs	# queries	sparsity
retrieval	MED	7,014	1,033	30	0.735
datasets	CRAN	3,763	1,398	225	1.412

Med dataset.

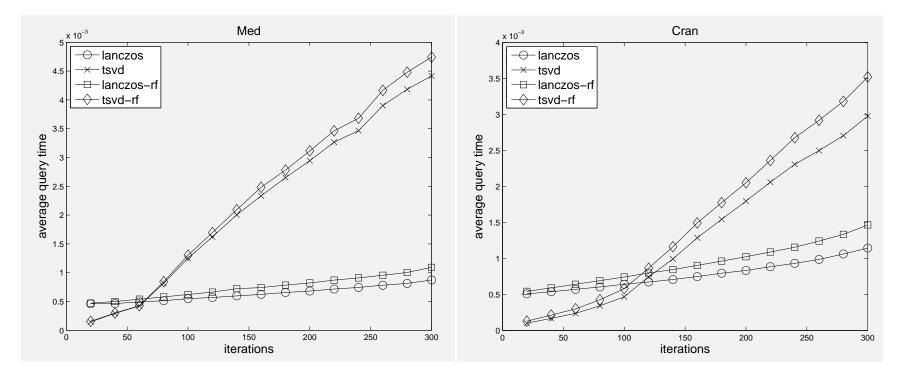
Cran dataset.



Kalamata, 09-05-2008 p. 23

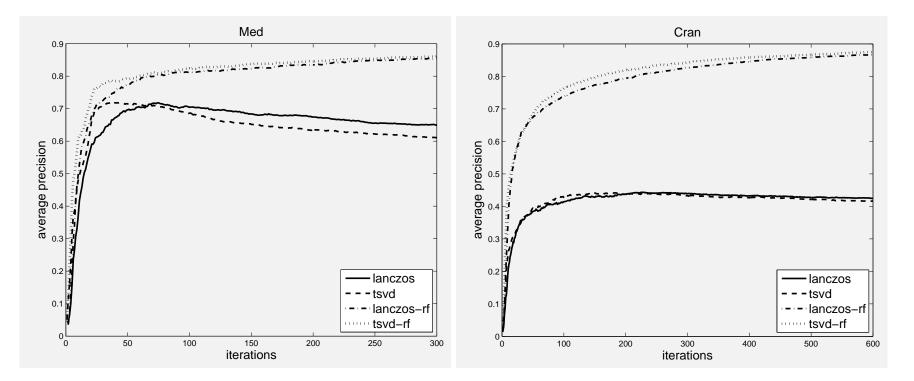
Med dataset

Cran dataset.



Med dataset

Cran dataset



Retrieval precision comparisons

In summary:

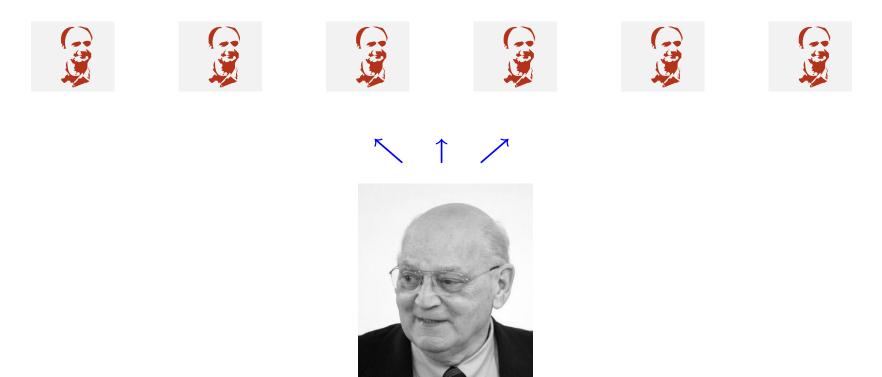
Results comparable to those of SVD ...

> .. at a much lower cost. [However not for the same dimension k] Thanks:

► Helpful tools and datasets widely available. We used TMG [developed at the U. of Patras (D. Zeimpekis, E. Gallopoulos)]

Problem 2: Face Recognition – background

Problem: We are given a database of images: [arrays of pixel values]. And a test (new) image.



Question: Does this new image correspond to one of those in the database?

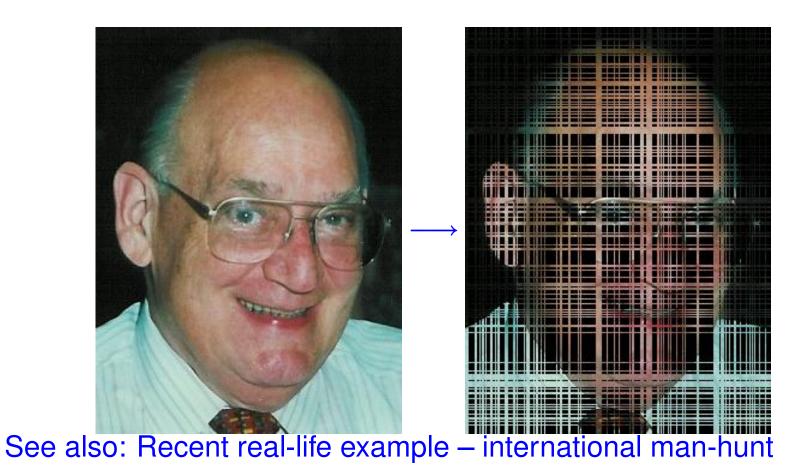
Different positions, expressions, lighting, ..., situations :



Common approach: eigenfaces – Principal Component Analysis technique

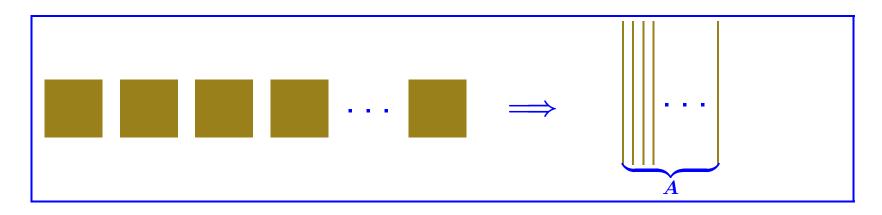
Example: Occlusion. See recent paper by John Wright et al.

Right: 50% pixels randomly changed



Eigenfaces

- Consider each picture as a one-dimensional colum of all pixels
- Put together into an array A of size $\#_pixels \times \#_images$.



- Do an SVD of A and perform comparison with any test image in low-dim. space
- Similar to LSI in spirit but data is not sparse.
- *Idea:* replace SVD by Lanczos vectors (same as for IR)

Tests: Face Recognition

Tests with 2 well-known data sets:

ORL 40 subjects, 10 sample images each – example:



of pixels : 112×92 TOT. # images : 400

AR set 126 subjects – 4 facial expressions selected for each [natural, smiling, angry, screaming] – example:



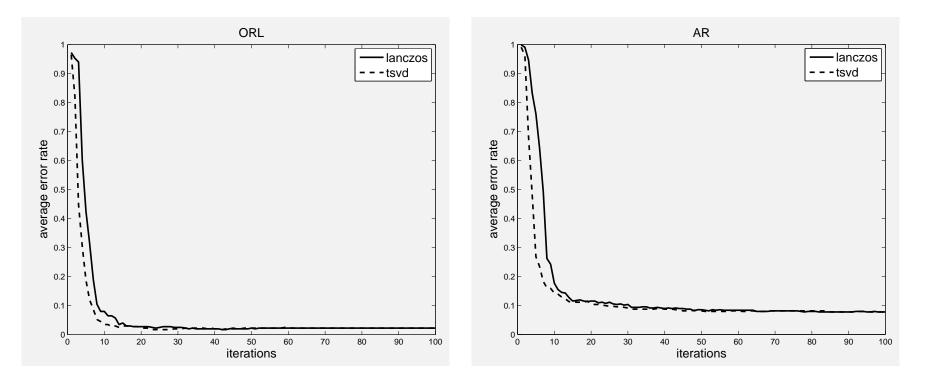
of pixels : 112×92 # TOT. # images : 504

Tests: Face Recognition

Recognition accuracy of Lanczos approximation vs SVD

ORL dataset

AR dataset



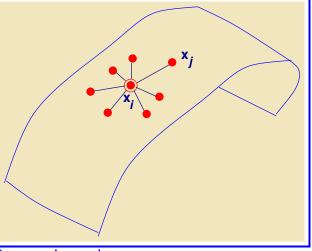
Vertical axis shows average error rate. Horizontal = Subspace dimension

GRAPH-BASED TECHNIQUES

Laplacean Eigenmaps (Belkin-Niyogi-02)

- Not a linear (projection) method but a Nonlinear method
- Starts with k-nearest-neighors graph
- Defines the graph Laplacean L = D W. Simplest:

$$D = ext{diag}(deg(i)); \hspace{1em} w_{ij} = \left\{egin{array}{cc} 1 \hspace{1em} ext{if} \hspace{1em} j \in N_i \ 0 \hspace{1em} ext{else} \end{array}
ight.$$



with N_i = neighborhood of i (excl. i); $deg(i) = |N_i|$

A few properties of graph Laplacean matrices

 \blacktriangleright Let L = any matrix s.t. L = D - W, with $D = diag(d_i)$ and

$$w_{ij} \geq 0, \qquad d_i ~=~ \sum_{j
eq i} w_{ij}$$

Property 1: for any $x \in \mathbb{R}^n$:

$$x^ op L x = rac{1}{2}\sum_{i,j} w_{ij} |x_i-x_j|^2$$

Property 2: (generalization) for any $Y \in \mathbb{R}^{d \times n}$:

$$\mathsf{Tr}\left[oldsymbol{Y} L oldsymbol{Y}^ op
ight] = rac{1}{2} \sum_{i,j} w_{ij} \| y_i - y_j \|^2$$

Property 3: For the particular $L = I - \frac{1}{n} \mathbf{1} \mathbf{1}^{\top}$

 $XLX^{ op} = ar{X}ar{X}^{ op} = = n imes ext{Covariance matrix}$

[Proof: 1) L is a projector: $L^{\top}L = L^2 = L$, and 2) $XL = \overline{X}$]

- > Consequence-1: PCA equivalent to maximizing $\sum_{ij} \|y_i y_j\|^2$
- Consequence-2: what about replacing trivial L with something else? [viewpoint in Koren-Carmel'04]

Property 4: (Graph partitioning) If x is a vector of signs (± 1) then

 $x^{\top}Lx = 4 \times$ ('number of edge cuts')

edge-cut = pair (i, j) with $x_i \neq x_j$

Consequence: Can be used for partitioning graphs, or 'clustering' [take $p = sign(u_2)$, where $u_2 = 2nd$ smallest eigenvector..]

Return to Laplacean eigenmaps approach

Laplacean Eigenmaps *minimizes*

 $\mathcal{F}_{EM}(Y) = \sum_{i,j=1}^n w_{ij} \|y_i - y_j\|^2$ subject to $YDY^ op = I$.

Notes:

1. Motivation: if $||x_i - x_j||$ is small (orig. data), we want $||y_i - y_j||$ to be also small (low-D data)

- 2. Note Min instead of Max as in PCA [counter-intuitive]
- 3. Above problem uses original data indirectly through its graph

Problem translates to:

$$egin{aligned} \min & \operatorname{Tr} \left[Y(D-W)Y^{ op}
ight] \ & Y \in \mathbb{R}^{d imes n} \ & YD \; Y^{ op} = I \end{aligned}$$

Solution (sort eigenvalues increasingly):

$$(D-W)u_i = \lambda_i D u_i \ ; \quad y_i = u_i^ op; \quad i=1,\cdots,d$$

Note: an n × n sparse eigenvalue problem [In 'sample' space]
 Note: can assume D = I. Amounts to rescaling data. Problem becomes

$$(I-W)u_i=\lambda_i u_i \ ; \quad y_i=u_i^ op; \quad i=1,\cdots,d$$

Intuition:

Graph Laplacean and 'unit' Laplacean are very different: one involves a sparse graph (More like a discr. differential operator). The other involves a dense graph. (More like a discr. integral operator). They should be treated as the inverses of each other.

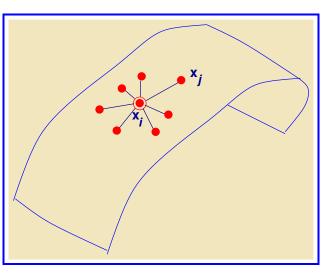
Viewpoint confirmed by what we learn from Kernel approach

Locally Linear Embedding (Roweis-Saul-00)

LLE is very similar to Eigenmaps. Main differences:
1) Graph Laplacean matrix is replaced by an 'affinity' graph
2) Objective function is changed: want to preserve graph

1. Graph:Each x_i is written as a convexcombination of its k nearest neighbors: $x_i \approx \Sigma w_{ij} x_j, \quad \sum_{j \in N_i} w_{ij} = 1$ \blacktriangleright Optimal weights computed ('local calculation') by minimizing

$$\|x_i - \Sigma w_{ij} x_j\|$$
 for $i=1,\cdots,n$



2. Mapping:

The y_i 's should obey the same 'affinity' as x_i 's \rightsquigarrow

Minimize:

$$\sum_{i} \left\| y_i - \sum_{j} w_{ij} y_j \right\|^2$$
 subject to: $Y\mathbf{1} = 0, \quad YY^{ op} = I$

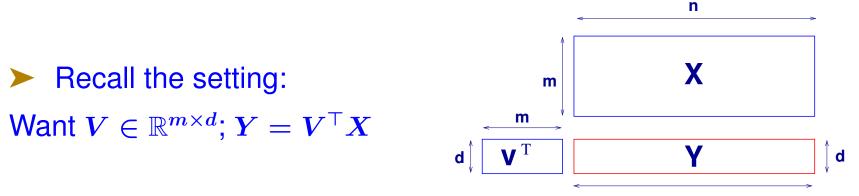
Solution:

$$(I-W^ op)(I-W)u_i=\lambda_i u_i; \qquad y_i=u_i^ op$$
 .

 $(I - W^{\top})(I - W)$ replaces the graph Laplacean of eigenmaps

Locally Preserving Projections (He-Niyogi-03)

LPP is a linear dimensionality reduction technique



Starts with the same neighborhood graph as Eigenmaps: $L \equiv D - W =$ graph 'Laplacean'; with $D \equiv diag(\{\Sigma_i w_{ij}\})$.

Optimization problem is to solve

$$\min_{\substack{Y \in \mathbb{R}^{d imes n}, \; YDY^ op = I}} \quad \Sigma_{i,j} w_{ij} \left\|y_i - y_j
ight\|^2, \; \; Y = V^ op X.$$

> Difference with eigenmaps: Y is a projection of X data

Solution (sort eigenvalues increasingly)

$$XLX^ op v_i = \lambda_i XDX^ op v_i \quad y_{i,:} = v_i^ op X_i$$

Note: essentially same method in [Koren-Carmel'04] called 'weighted PCA' [viewed from the angle of improving PCA]

ONPP (Kokiopoulou and YS '05)

- Orthogonal Neighborhood Preserving Projections
- Can be viewed as a linear version of LLE
- Uses the same graph as LLE. Objective: preserve the affinity graph (as in LEE) *but* by means of an orthogonal projection
 Objective function

Objective function

 $\Phi(Y) = \Sigma_i \|y_i - \Sigma_j w_{ij} y_j\|^2$ Constraint: $Y = V^\top X, V^\top V = I$

Notice that

 $\Phi(Y) = \|Y - YW^{ op}\|_F^2 = \cdots = \operatorname{Tr} \left[V^{ op}X(I - W^{ op})(I - W)X^{ op}V
ight]$

Resulting problem:

$$\min_{\substack{V \in \mathbb{R}^{m \times d}; \\ V^{\top}V = I}} \mathbf{Tr} \left[V^{\top} \underbrace{X(I - W^{\top})(I - W)X^{\top}}_{M} V \right]$$

Solution: Columns of V = eigenvectors of M associated with smallest d eigenvalues

Can be computed as d lowest left singular vectors of

 $X(I-W^{ op})$

A unified view

Method	Object. (min)	Constraint
PCA/MDS	$Tr\left[V^ op X(-I+ee^ op)X^ op V ight]$	$V^{ op}V = I$
LLE	$Tr\left[oldsymbol{Y}(I-W^ op)(I-W)oldsymbol{Y}^ op ight]$	$YY^{ op} = I$
Eigenmaps	$Tr\left[oldsymbol{Y}(oldsymbol{I}-oldsymbol{W})oldsymbol{Y}^{ op} ight]$	$YY^{ op} = I$
LPP	$Tr\left[oldsymbol{V}^ opoldsymbol{X}(oldsymbol{I}-oldsymbol{W})oldsymbol{X}^ opoldsymbol{V} ight]$	$V^ op X X^ op V = I$
ONPP	$Tr\left[m{V}^ opm{X}m{X}(m{I}-m{W}^ op)(m{I}-m{W})m{X}^ opm{V} ight]$	$V^{ op}V = I$
LDA	$Tr\left[V^ op X (I-H) X^ op V ight]$	$V^{ op}XX^{ op}V = I$

Let M = I - W = a Laplacean matrix $(-I + ee^{\top}$ for PCA/MDS); or the LLE matrix $(I - W)(I - W^{\top})$, or geodesic distance matrix (ISOMAP).

All techniques lead to one of two types of problems

First type is:
$$egin{array}{ccc} \min & \mathsf{Tr} & [YMY^{ op}] \ Y \in \mathbb{R}^{d imes n} \ YY^{ op} = I \end{array}$$

- Y obtained from solving an eigenvalue problem
- LLE, Eigenmaps (normalized), ..

And the second type is:

 $egin{array}{ccc} \min & \mathsf{Tr} \; ig[V^ op X M X^ op V ig] \ V \in \mathbb{R}^{m imes d} \ V^ op \; G \; V = I \end{array}$

- > G is either the identity matrix or XDX^{\top} or XX^{\top} .
- > Low-Dim. data : $Y = V^{\top}X$

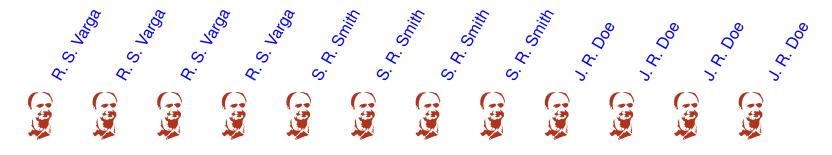
Important observation: 2nd is just a projected version of the 1st,

i.e., approximate eigenvectors are sought in Span $\{X\}$ [Rayleigh-Ritz procedure]

- > Problem is of dim. m (dim. of data) not n (# of samples).
- This difference can be mitigated by resorting to Kernels..

Graph-based methods in a supervised setting

Subjects of training set are known (labeled). Q: given a test image (say) find its label.





Question: Find label (best match) for test image.

Methods can be adapted to supervised mode by building the graph to take into account class labels. Idea is simple: Build G so that nodes in the same class are neighbors. If c = # classes, G will consist of c cliques.

Matrix W will be block-diagonal

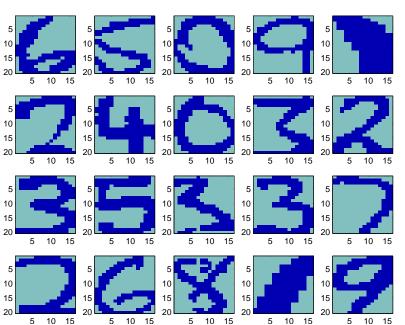
$$W=diag(W_1,W_2,\cdots,W_c)$$

- Easy to see that rank(W) = n c.
- Can be used for LPP, ONPP, etc..

TIME FOR A MATLAB DEMO

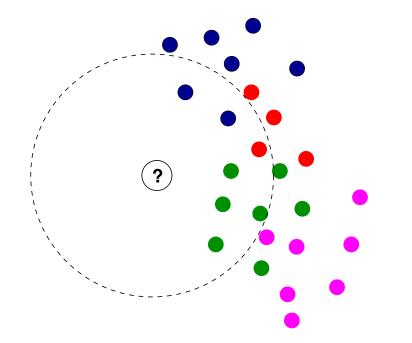
Supervised learning experiments: digit recognition

- Set of 390 images of digits (39 of each digit)
- Each picture has $20 \times 16 = 320 \frac{5}{10}$ pixels.
- Select any one of the digits ¹⁰/₂₀
 and try to recognize it among the ⁵/₁₀
 389 remaining images ²⁰
- Methods: KNN, PCA, LPP, ONPP



One word about KNN-classifiers

- Simple idea of 'vote' get k nearest neighbors.
- Assigned label = 'most common label among these neibhbors'



MULTILEVEL METHODS

Multilevel techniques

Divide and conquer paradigms as well as multilevel methods in the sense of 'domain decomposition'

Main principle: very costly to do an SVD [or Lanczos] on the whole set. Why not find a smaller set on which to do the analysis – without too much loss?

Tools used: graph coarsening, divide and conquer –

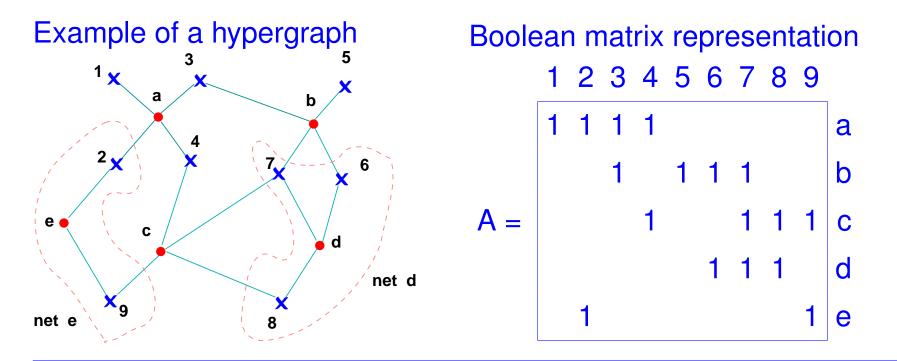
Multilevel techniques: Hypergraphs to the rescue

General idea: Given $X = [x_1, \cdots, x_n] \in \mathbb{R}^{m \times n}$ find another set ('coarsened set') $\hat{X} = [\hat{x}_1, \cdots, \hat{x}_k] \in \mathbb{R}^{m \times k}$

- > \hat{X} should be a good representative of X –
- \blacktriangleright then find projector from \mathbb{R}^m to \mathbb{R}^d based on this subset
- Main tool used: graph coarsening.
- We will describe hypergraph-based techniques

Hypergraphs

- A hypergraph H = (V, E) is a generalization of a graph
- \blacktriangleright V = set of vertices V
- \blacktriangleright E = set of hyperedges. Each $e \in E$ is a nonempty subset of V
- > Standard undirected graphs: each e consists of two vertices.
- degree of e = |e|
- > degree of a vertex v = number of hyperedges e s.t. $x \in e$.
- Two vertices are *neighbors* if there is a hyperedge connecting them



Canonical hypergraph representation for sparse data (e.g. text)

Hypergraph Coarsening

Coarsening a hypergraph H = (V, E) means finding a 'coarse' approximation $\hat{H} = (\hat{V}, \hat{E})$ to H with $|\hat{V}| < |V|$, which tries to retain as much as possible of the structure of the original hypergraph

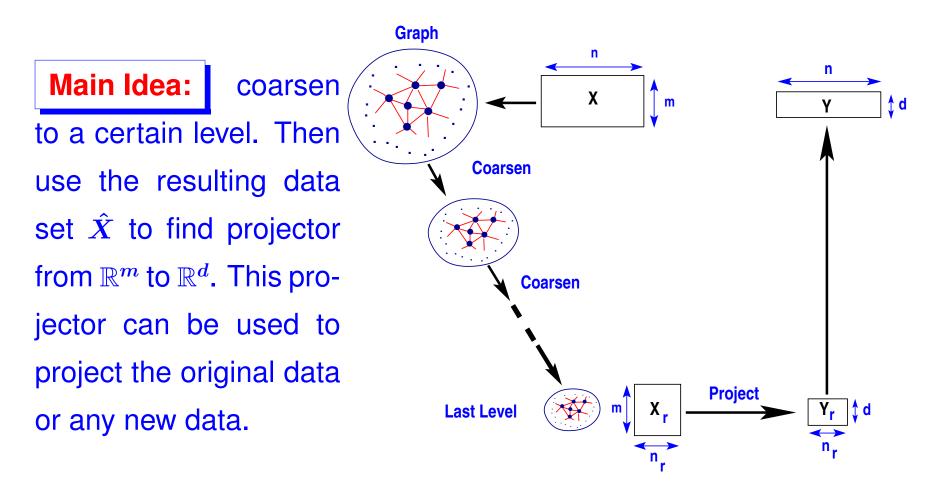
Idea: repeat coarsening recursively.

• •

- Result: succession of smaller hypergraphs which approximate the original graph.
- Several methods exist. We use 'matching', which successively merges pairs of vertices
- Used in most graph partitioning methods: hMETIS, Patoh, zoltan,

Algorithm successively selects pairs of vertices to merge – based on measure of similarity of the vertices.

Application: Multilevel Dimension Reduction



Main gain: Dimension reduction is done with a much smaller set. Hope: not much loss compared to using whole data

Application to text mining

- Recall common approach:
- 1. Scale data [e.g. TF-IDF scaling:]
- 2. Perform a (partial) SVD on resulting matrix $X \approx U_d \Sigma_d V_d^T$
- 3. Process query by same scaling (e.g. TF-IDF)
- 4. Compute similarities in *d*-dimensional space: $s_i = \langle \hat{q}, \hat{x}_i \rangle / \|\hat{q}\| \|\hat{x}_i\|$ where $[\hat{x}_1, \hat{x}_2, \dots, \hat{x}_n] = V_d^T \in \mathbb{R}^{d \times n}$; $\hat{q} = \Sigma_d^{-1} U_d^T \bar{q} \in \mathbb{R}^d$

Multilevel approach: replace SVD (or any other dim. reduction) by dimension reduction on coarse set. Only difference: TF-IDF done on the coarse set not original set.

Tests

Three public data sets used for experiments: Medline, Cran and NPL (cs.cornell.edu)

Coarsening to a max. of 4 levels.

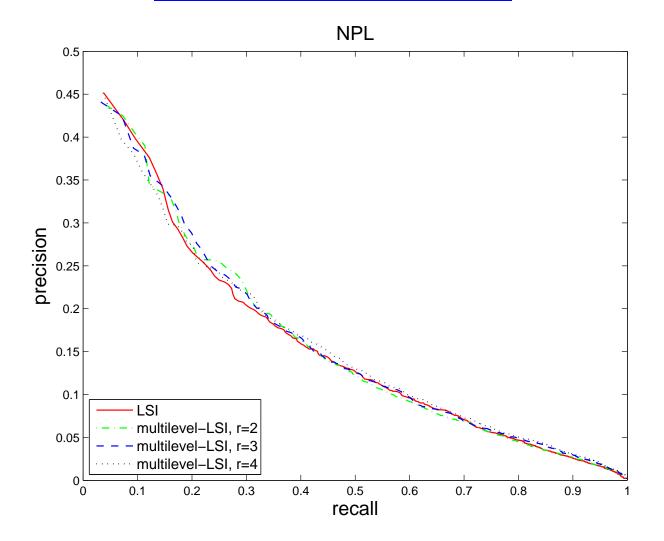
Data set	Medline	Cran	NPL
# documents	1033	1398	11429
# terms	7014	3763	7491
sparsity (%)	0.74%	1.41%	0.27%
# queries	30	225	93
avg. # rel./query	23.2	8.2	22.4

Results with NPL

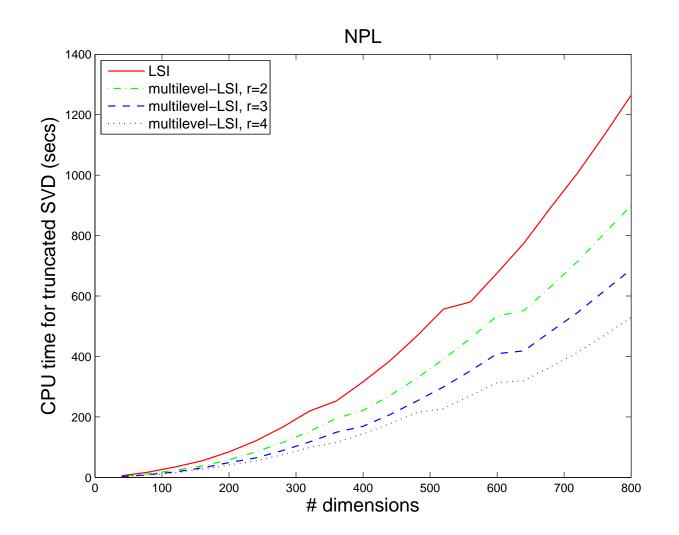
Statistics

Level	coarsen.	#	optimal	optimal avg.
	time	doc.	# dim.	precision
#1	N/A	11429	736	23.5%
#2	3.68	5717	592	23.8%
#3	2.19	2861	516	23.9%
#4	1.50	1434	533	23.3%

Precision-Recall curves



CPU times for preprocessing (Dim. reduction part)



Conclusion

So how is this related to intitial title of "efficient algorithms in data mining"?

Answer: All these eigenvalue problems are not cheap to solve..

... and cost issue does not seem to bother practitioners too much for now..

- Ingredients that will become mandatory:
 - 1 Avoid the SVD
 - *2* Fast algorithms that do not sacrifice quality.
 - 3 In particullar: Multilevel approaches
 - 4 Multilinear algebra [tensors]